

An alternative solution of Diatomic Molecules

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Abstract

The spectrum of r^{-1} and r^{-2} type potentials of diatomic molecules in radial Schrödinger equation are calculated by using the formalism of asymptotic iteration method. The alternative method is used to solve eigenvalues and eigenfunctions of Mie potential, Kratzer-Fues potential, Coulomb potential, and Pseudoharmonic potential by determining the α , β , γ and σ parameters.

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I. INTRODUCTION

In the last few decades, there has been raised a great deal of interest in many branches of physics in order to calculate the energy eigenvalues and eigenfunctions of diatomic molecules [1]. The most important analytical methods which have been used in literature to solve these studies are supersymmetry (SUSY) [2], Nikiforov-Uvarov (NU) method [3], Pekeris approximation [4], variational method [5], hypervirial perturbation method [6], shifted $1/N$ expansion (SE) and the modified shifted $1/N$ expansion (MSE) [7], exact quantization rule (EQR) [8], perturbative formalism [9, 10], polynomial solution [11], wave function ansatz method [12], path integral [13], Lie algebraic method [14, 15], Fourier Grid Hamiltonian method [16], and asymptotic iteration method (AIM) [17] to solve the radial Schrödinger equation exactly.

Among these methods, AIM which was developed by H.Ciftci in 2003 to solve the Schrödinger like second order differential equation, has been used in many field of physics due to simplicity in obtaining the energy eigenvalues and corresponding eigenfunctions [18, 19]. To apply the method, the asymptotic wavefunction form should be proposed after substituting the potential in Schrödinger equations. Then the AIM is applied to calculate the spectrum of potentials. But in this study, we propose an asymptotic wavefunction to the radial Schrödinger equation before substituting the potential function. This yields to write a general asymptotic form of Schrödinger equation which is amenable to apply the termination condition in AIM. The transformed radial Schrödinger equation is applied to Mie potential, Kratzer-Fues potential, Coulomb potential, and Pseudoharmonic potential. The energy eigenvalues and eigenfunctions satisfy the corresponding results in literature.

The organization of this study is as follows: the general Hamiltonian for diatomic is introduced in the Section II. A general description of AIM is outlined in Section III. Section IV is devoted to proposed form of AIM with applications. Finally, Section V is devoted to a conclusion.

II. FORMALISM OF THE PROPOSED METHOD FOR DIATOMIC MOLECULES

The Hamiltonian operator for diatomic molecules with spherically symmetric potential which means depends only on r ; separation distance between two molecules, not θ or ϕ , takes the form [20]

$$\hat{H} = \left\{ \frac{1}{r} \frac{d}{dr} \left(r^2 \frac{d}{dr} \right) + \frac{\hat{L}^2}{2\mu r^2} + V(r) \right\} \quad (1)$$

where V is the potential, \hat{L} is the angular momentum operator and $\mu = m_1 m_2 / m_1 + m_2$ is called the reduced mass; m_1 and m_2 are the mass of molecules 1 and 2, respectively. By using the separation of variable for wavefunction

$$\Psi(r, \theta, \phi) = R_{n\ell}(r) Y_\ell^m(\theta, \phi) \quad (2)$$

The Schrödinger equation by using Eq.(1) and Eq.(2) turns into

$$\left\{ \frac{1}{r} \frac{d}{dr} \left(r^2 \frac{d}{dr} \right) + \frac{\ell(\ell+1)\hbar^2}{2\mu r^2} + V(r) \right\} R_{n\ell}(r) = E_n R_{n\ell}(r) \quad (3)$$

where E is the energy, n is the radial quantum number, ℓ is the angular momentum quantum number and $Y_\ell^m(\theta, \phi)$ is an eigenfunction of \hat{L}^2 with eigenvalue $\ell(\ell+1)\hbar^2$. Moreover, the angular part of the wavefunction Y_ℓ^m can be canceled from this equation because all terms contained one such factor, r . The angular momentum L is conserved that will not change with time for such potentials. This reduces the Hamiltonian to one dimensional effective system for the radial part of the wavefunction $R_{n\ell}$ as seen in Eq.(3)[21].

After rearranging the Eq.(3), we get

$$\frac{d^2 R_{n\ell}(r)}{dr^2} + \frac{2}{r} \frac{dR_{n\ell}(r)}{dr} + \frac{2\mu}{\hbar^2} \left[E_n - V(r) - \frac{\ell(\ell+1)\hbar^2}{2\mu r^2} \right] R_{n\ell}(r) = 0 \quad (4)$$

If we make the following substitution

$$\rho = 2\alpha r^k \quad (5)$$

where α and k are constants. In terms of this variable the Eq.(4) becomes,

$$\frac{d^2 R_{n\ell}(\rho)}{d\rho^2} + \frac{1}{\rho} \left(\frac{k+1}{k} \right) \frac{dR_{n\ell}(\rho)}{d\rho}$$

$$+ \frac{2\mu}{\hbar^2} \left(\frac{1}{4\alpha^2 k^2} \right) \left(\frac{\rho}{2\alpha} \right)^{-\frac{2(k-1)}{k}} \left[E_n - V(r) - \frac{\ell(\ell+1)\hbar^2}{2\mu r^2} \right] R_{n\ell}(\rho) = 0 \quad (6)$$

whose solution gives the energy levels of the system by using the Laguerre functions. The wavefunction $R_{n\ell}(\rho)$ can be given by in this form [22]

$$R(\rho) = \rho^\gamma \exp\left[-\frac{\rho}{2}\right] G(\rho) \quad (7)$$

where γ is a constant and $G(\rho)$ represents Laguerre function. We substitute this equation into the Eq.(6) and make some algebra to get the equation for $G(\rho)$. The general expression for this function can be written as

$$\begin{aligned} & G''(\rho) + \left[\left(2\gamma + \frac{k+1}{k} \right) \frac{1}{\rho} - 1 \right] G'(\rho) \\ & + \left\{ \frac{1}{4} - \left(\gamma + \frac{k+1}{2k} \right) \frac{1}{\rho} + \gamma(\gamma-1) + \frac{k+1}{k} \frac{1}{\rho^2} \right\} G(\rho) \\ & + \frac{2\mu}{\hbar^2} \left(\frac{1}{4\alpha^2 k^2} \right) \left(\frac{\rho}{2\alpha} \right)^{-\frac{2(k-1)}{k}} \left[E_n - V(r) - \frac{\ell(\ell+1)\hbar^2}{2\mu r^2} \right] G(\rho) = 0 \end{aligned} \quad (8)$$

If $k = 1$ or $\rho = 2\alpha r$, the general expression, Eq.(8) becomes

$$\begin{aligned} & G''(\rho) + \left[\frac{2(\gamma+1)}{\rho} - 1 \right] G'(\rho) + \\ & \left\{ \frac{1}{4} - \frac{(\gamma+1)}{\rho} + \frac{\gamma(\gamma+1)}{\rho^2} + \frac{2\mu}{\hbar^2} \left(\frac{1}{4\alpha^2} \right) \left[E_n - V(r) - \frac{\ell(\ell+1)\hbar^2}{2\mu r^2} \right] \right\} G(\rho) = 0 \end{aligned} \quad (9)$$

If $k = 2$ or $\rho = 2\alpha r^2$, the general expression, Eq.(8) becomes

$$\begin{aligned} & G''(\rho) + \left[\left(2\gamma + \frac{3}{2} \right) \frac{1}{\rho} - 1 \right] G'(\rho) + \\ & \left\{ \frac{1}{4} - \frac{(\gamma + \frac{3}{4})}{\rho} + \frac{\gamma(\gamma + \frac{1}{2})}{\rho^2} + \frac{\mu}{\hbar^2} \left(\frac{1}{4\alpha\rho} \right) \left[E_n - V(r) - \frac{\ell(\ell+1)\hbar^2}{2\mu r^2} \right] \right\} G(\rho) = 0 \end{aligned} \quad (10)$$

Now we will find the analytical solutions of the Eq.(8) for diatomic potentials with any angular momentum. The Eq.(8) can be transformed into a second order differential equation

form for the corresponding potentials. The transformed differential equations are solved within the framework of the asymptotic iteration method. We apply our formalism to several important diatomic potentials and obtain the energy eigenvalues and the corresponding eigenfunctions [23].

III. ASYMPTOTIC ITERATION METHOD

The starting point of AIM is to consider the following second order homogeneous differential equation:

$$y''(x) = \lambda_0 y'(x) + s_0 y(x), \quad (11)$$

where λ_0 and s_0 are functions and $y'(x)$ and $y''(x)$ denotes derivative of y with respect to x . It is easy to show that $(n+2)^{th}$ derivative of the function $y(x)$ can be written as

$$y^{(n+2)}(x) = \lambda_n y'(x) + s_n y(x) \quad (12)$$

where λ_n and s_n are given by the recurrence relations

$$\lambda_n = \lambda'_{n-1} + s_{n-1} + \lambda_{n-1} \lambda_0, \quad s_n = s'_{n-1} + \lambda_{n-1} s_0 \quad (13)$$

If we have, for sufficiently large n ,

$$\frac{\lambda_n}{s_n} = \frac{\lambda_{n-1}}{s_{n-1}} = \alpha(x) \quad (14)$$

then the solution of Eq. (11) can be written as below

$$y(x) = \exp\left(-\int^x \alpha dt\right) \left[C_1 + C_2 \int^x \exp\left(\int^t (\lambda_0 + 2\alpha) d\tau\right) dt \right] \quad (15)$$

In calculating the parameters in Eq. (13), for $n = 0$, we take the initial conditions as $\lambda_{-1} = 1$ and $s_{-1} = 0$ [24] and $\Delta_n(x) = 0$ for

$$\Delta_n(x) = \lambda_n(x) s_{n-1}(x) - \lambda_{n-1}(x) s_n(x) \quad (16)$$

where $\Delta_n(x)$ is the termination condition method in Eq. (14).

In order to find the corresponding energy eigenfunctions, the following wave function generator is used ([25],[26])

$$f_n(x') = \int \frac{\lambda_n(x')}{s_n(x')} dx' \quad (17)$$

where x' is a variable and n is the radial quantum number.

IV. APPLICATION OF PROPOSED METHOD IN DIATOMIC POTENTIALS

A. Mie Potential

Mie potential is the intermolecular pair potential which was proposed by Gustav Mie (1903) who was first to introduce an attractive term and a repulsive one. The attractive term is the van der Waals interaction potential which varies with the inverse power of the distance between molecules [27]. The superposition of these terms produces an effective potential pocket and the form of this pocket is very important for the correct energy eigenvalues. For the Mie potential $r \rightarrow 0$, $V(r) \rightarrow \infty$ because there is internuclear repulsion. As $r \rightarrow \infty$, $V(r) \rightarrow 0$, i.e. the molecule decomposes [26].

Generally one can define the Mie-type potential as ([28],[29])

$$V(r) = \epsilon \left[\frac{p}{q-p} \left(\frac{a}{r} \right)^q - \frac{q}{q-p} \left(\frac{a}{r} \right)^p \right] \quad (18)$$

where ϵ is the interaction energy between two atoms in a molecular system at distance a , q and p are constants which $q > p$ is always satisfied. The solution of the one-dimensional Mie potential with $q = 2p$ combination by choosing the special case $p = 1$ takes the following form

$$V(r) = V_0 \left[\frac{1}{2} \left(\frac{a}{r} \right)^2 - \left(\frac{a}{r} \right) \right] \quad (19)$$

where $V_0 = 2\epsilon p$ is the dissociation energy and a is the equilibrium internuclear distance. Inserting this potential equation into the general expression for $k = 1$, the Eq.(9) can be written

$$\begin{aligned} G''(\rho) + \left[\frac{2(\gamma+1)}{\rho} - 1 \right] G'(\rho) + \left\{ \frac{1}{4} - \frac{(\gamma+1)}{\rho} + \frac{\gamma(\gamma+1)}{\rho^2} \right\} G(\rho) \\ + \left\{ \frac{2\mu E_n}{\hbar^2 4\alpha^2} - \frac{\mu V_0}{\hbar^2} \frac{a^2}{4\alpha^2 r^2} + \frac{2\mu V_0}{\hbar^2} \frac{a}{4\alpha^2 r} - \frac{\ell(\ell+1)}{4\alpha^2 r^2} \right\} G(\rho) = 0 \end{aligned} \quad (20)$$

Rearranging the Eq.(20) with constants, we get

$$\begin{aligned} G''(\rho) + \left[\frac{2(\gamma+1)}{\rho} - 1 \right] G'(\rho) \\ + \left\{ \frac{1}{4} - \frac{(\gamma+1)}{\rho} + \frac{\beta}{\alpha\rho} + \frac{\gamma(\gamma+1)}{\rho^2} - \frac{\ell(\ell+1)}{\rho^2} - \frac{\beta a}{\rho^2} - \frac{1}{4} \right\} G(\rho) = 0 \end{aligned} \quad (21)$$

where

$$\alpha^2 = -\frac{2\mu E_n}{\hbar^2}$$

$$\beta = \frac{\mu V_0 a}{\hbar^2}$$

To find the γ term, we make the following assumption

$$\frac{\gamma(\gamma+1)}{\rho^2} - \frac{[\ell(\ell+1) + \beta a]}{\rho^2} = 0 \quad (22)$$

and the solutions of this equation are obtained as

$$\gamma_{1,2} = \frac{1}{2} \left(-1 \mp \sqrt{1 + 4\sigma} \right). \quad (23)$$

where $\sigma = \ell(\ell+1) + \beta a$ is a constant. The positive term must be chosen for appropriate solutions of eigenvalues [28]. For simplicity we use $\gamma+1 = \sigma/\rho$, and we get the general expression in this form

$$G''(\rho) = \left[1 - \frac{2\sigma}{\gamma\rho} \right] G'(\rho) + \left\{ \frac{\sigma}{\gamma\rho} - \frac{\beta}{\alpha\rho} \right\} G(\rho) = 0 \quad (24)$$

The Eq.(24) is a homogeneous linear second-order differential equation, it can be solved by the AIM where

$$\lambda_0 = 1 - \frac{2\sigma}{\gamma\rho}$$

$$s_0 = \frac{\sigma}{\gamma\rho} - \frac{\beta}{\alpha\rho} \quad (25)$$

If we use the termination condition of the AIM in Eq.(16), the energy eigenvalues are obtained as follows

$$\lambda_1 s_0 - s_1 \lambda_0 = 0 \implies E_0 = -\frac{\hbar^2 \beta^2 \gamma^2}{2\mu \sigma^2}$$

$$\lambda_2 s_1 - s_2 \lambda_1 = 0 \implies E_1 = -\frac{\hbar^2 \beta^2 \gamma^2}{2\mu (\gamma + \sigma)^2}$$

$$\lambda_3 s_2 - s_3 \lambda_2 = 0 \implies E_2 = -\frac{\hbar^2 \beta^2 \gamma^2}{2\mu (2\gamma + \sigma)^2}$$

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which can be generalized as following

$$E_n = -\frac{\hbar^2}{2\mu} (2\beta)^2 [2n + 1 + \sqrt{1 + 4\sigma}]^{-2} \quad (26)$$

Here, n denotes the radial quantum number; $n = 0, 1, 2, \dots$. Using the Eq.(17), we can write the corresponding eigenfunctions

$$\begin{aligned} f_0(\rho) &= 1 \\ f_1(\rho) &= 2 + 2\gamma - \rho \\ f_2(\rho) &= 6 + 4\gamma^2 + 10\gamma - \gamma\rho - 6\rho + \rho^2 \\ f_3(\rho) &= 24 + 52\gamma + 36\gamma^2 + 8\gamma^3 - 36\rho - 42\gamma\rho - 12\gamma^2\rho + 12\rho^2 + 6\gamma\rho^2 - \rho^3 \\ &\dots\dots\dots \end{aligned}$$

It is understood from the results given above that we can write the general formula for $f_n(\rho)$ as Laguerre function using Eq.(23)

$$f_n(\rho) = L_n^{\sqrt{1+4\sigma}}(\rho) \quad (27)$$

Thus we can write the radial wavefunction as below substituting the results in Eq.(5) and Eq.(27) into the Eq.(7)

$$R_{n\ell}(\rho) = \rho^{\frac{1}{2}(-1+\sqrt{1+4\sigma})} \exp[-i\varepsilon r] L_n^{\sqrt{1+4\sigma}}(2i\varepsilon r) \quad (28)$$

where $\varepsilon^2 = 2\mu E/\hbar^2$. They are exactly same as with the eigenvalue and eigenfunction equations obtained in [28]

B. Kratzer-Fues potential

The Kratzer-Fues potential is a Mie type potential and it is modified by adding a D_e term to potential in the Eq.(19). A new type of this potential is called the modified Kratzer potential and it is given by ([30],[29],[31])

$$V(r) = D_e \left[\frac{r - r_e}{r} \right]^2 = D_e \left[1 - 2\frac{r_e}{r} + \frac{r_e^2}{r^2} \right] \quad (29)$$

where D_e is the interaction energy between two atoms in a molecular system at equilibrium distance r_e . And the general expression for $k = 1$ in Eq.(9) can be written with this potential

$$\begin{aligned}
& G''(\rho) + \left[\frac{2(\gamma + 1)}{\rho} - 1 \right] G'(\rho) \\
& + \left\{ \frac{1}{4} - \frac{(\gamma + 1)}{\rho} + \frac{\gamma(\gamma + 1)}{\rho^2} \right\} G(\rho) \\
& + \left\{ \frac{2\mu(E_n - D_e)}{\hbar^2 4\alpha^2} - \frac{\mu D_e}{\hbar^2} \frac{r_e^2}{4\alpha^2 r^2} + \frac{2\mu D_e}{\hbar^2} \frac{r_e}{4\alpha^2 r} - \frac{\ell(\ell + 1)}{4\alpha^2 r^2} \right\} G(\rho) = 0
\end{aligned} \tag{30}$$

The following equation is obtained by using the Eqs.(21,22,23)

$$G''(\rho) = \left[1 - \frac{2\sigma}{\gamma\rho} \right] G'(\rho) + \left\{ \frac{\sigma}{\gamma\rho} - \frac{\beta}{\alpha\rho} \right\} G(\rho) = 0 \tag{31}$$

where

$$\begin{aligned}
\alpha^2 &= -\frac{2\mu(E_n - D_e)}{\hbar^2} \\
\beta &= \frac{2\mu D_e r_e}{\hbar^2} \\
\gamma &= \frac{1}{2} \left(-1 + \sqrt{1 + 4\sigma} \right) \\
\sigma &= \ell(\ell + 1) + \beta r_e
\end{aligned}$$

Now, we reach to a position that the differential equation is suitable for applying AIM. Therefore, the energy eigenvalues of Eq.(31) should has a solution in the form of Eq.(26)

$$\varepsilon_n = -(2\beta)^2 [2n + 1 + \sqrt{1 + 4\sigma}]^{-2} \tag{32}$$

where $\varepsilon_n^2 = 2\mu(E_n - D_e)/\hbar^2$, ε is called energy spectrum. Using the wavefunction generator, we get the energy eigenfunction as in the Eq.(27). The Eq.(5) and the Eq.(7) give the following formula for the total radial wavefunction

$$R_{n\ell}(\rho) = \rho^{\frac{1}{2}(-1+\sqrt{1+4\sigma})} \exp\left[-\frac{\rho}{2}\right] L_n^{\sqrt{1+4\sigma}}(\rho) \tag{33}$$

which is exactly same as with the eigenvalue equation obtained in [30] through a proper choice of parameters.

C. Coulomb potential

The coulomb potential is an effective pair potential that describes the electrostatic interaction between electrically charged particles. This potential is given by

$$V(r) = -\frac{kZe^2}{r} \quad (34)$$

where r is the distance between two atoms, e is the electron charge, Z is the atomic number and $k = 1/4\pi\epsilon_0$ is a constant; ϵ_0 is the electrical permittivity of the space. By using the potential, the same expression for $k=1$ is obtained as in Eq.(24)

$$G''(\rho) = \left[1 - \frac{2\sigma}{\gamma\rho}\right] G'(\rho) + \left\{\frac{\sigma}{\gamma\rho} - \frac{\beta}{\alpha\rho}\right\} G(\rho) = 0 \quad (35)$$

where

$$\begin{aligned} \alpha^2 &= -\frac{2\mu E_n}{\hbar^2} \\ \beta &= \frac{\mu k Z e^2}{\hbar^2} \\ \gamma &= \frac{1}{2} \left(-1 + \sqrt{1 + 4\sigma}\right) \\ \sigma &= \ell(\ell + 1) \end{aligned}$$

Here for this potential $\gamma = \ell$ and in general we obtain the energy eigenvalues by changing the parameters in Eq.(26)

$$E_n = -\frac{\mu k^2 Z^2 e^4}{2\hbar^2 (n + \ell + 1)^2} \quad (36)$$

where n is the radial quantum number and ℓ is the angular momentum quantum number. We obtained the general formula of corresponding eigenfunctions for the Eq.(35) as Laguerre function in Eq.(27). Again by changing the parameters we can write the total radial wavefunction

$$R_{n\ell}(\rho) = N \rho^\ell \exp\left[-\frac{\rho}{2}\right] L_n^{2\ell+1}(\rho) \quad (37)$$

where N is a normalization constant and the total energy eigenvalues in Eq. (36) and the total wavefunction in (37) are exactly same as with the values that obtained in [23].

D. Pseudoharmonic potential

Pseudoharmonic potential can be considered as an intermediate potential between the harmonic oscillator potential and the Morse-type potentials, which are more realistic anharmonic potentials. The Pseudoharmonic potential is one of the exactly solvable potential and defines the real physical systems that have generally anharmonical properties [34]. It can be written as [35]

$$V(r) = V_0 \left[\frac{r}{r_0} - \frac{r_0}{r} \right]^2 = V_0 \left(\frac{r^2}{r_0^2} + \frac{r_0^2}{r^2} - 2 \right) \quad (38)$$

where V_0 is the dissociation energy and r_0 is the equilibrium intermolecular separation. Inserting the potential to the general expression for $k = 2$ in Eq.(10), the equation becomes

$$\begin{aligned} & G'''(\rho) + \left[\left(2\gamma + \frac{3}{2} \right) \frac{1}{\rho} - 1 \right] G'(\rho) \\ & + \left\{ \frac{1}{4} - \frac{(\gamma + \frac{3}{4})}{\rho} + \frac{\gamma(\gamma + \frac{1}{2})}{\rho^2} \right\} G(\rho) \\ & + \left\{ \frac{\mu(E_n + 2V_0)}{\hbar^2 4\alpha\rho} - \frac{\mu V_0}{\hbar^2 4\alpha\rho} \frac{r^2}{r_0^2} - \frac{\mu V_0}{\hbar^2 4\alpha\rho} \frac{r_0^2}{r^2} - \frac{\ell(\ell + 1)}{8\alpha\rho r^2} \right\} G(\rho) = 0 \end{aligned} \quad (39)$$

After rearranging this equation with following parameters

$$\begin{aligned} \alpha^2 &= \frac{\mu V_0}{2\hbar^2 r_0^2} \\ \beta &= \frac{\mu V_0 r_0^2}{2\hbar^2} \end{aligned}$$

we get

$$\begin{aligned} & G'''(\rho) + \left[\left(2\gamma + \frac{3}{2} \right) \frac{1}{\rho} - 1 \right] G'(\rho) \\ & + \left\{ \frac{1}{4} + \left[\frac{\mu(E_n + 2V_0)}{\hbar^2 4\alpha} - \gamma - \frac{3}{4} \right] \frac{1}{\rho} - \frac{1}{4} + \left[\gamma(\gamma + \frac{1}{2}) - \beta - \frac{\ell(\ell + 1)}{4} \right] \frac{1}{\rho^2} \right\} G(\rho) = 0 \end{aligned} \quad (40)$$

If we make the following assumption to find the γ term

$$\left[\gamma\left(\gamma + \frac{1}{2}\right) - \beta - \frac{\ell(\ell+1)}{4} \right] \frac{1}{\rho^2} = 0$$

The solution of this equation gives us the $\gamma = \frac{1}{4}(-1 + \sqrt{1 + 16\sigma})$ where $\sigma = \beta + \frac{\ell(\ell+1)}{4}$. The general expression becomes for this potential

$$G''(\rho) = \left[1 - \left(2\gamma + \frac{3}{2} \right) \frac{1}{\rho} \right] G'(\rho) + \left[\left(\gamma + \frac{3}{4} - \frac{\mu(E_n + 2V_0)}{2\hbar^2 2\alpha} \right) \frac{1}{\rho} \right] G(\rho) \quad (41)$$

By using the termination condition of AIM in Eq.(16) where

$$\begin{aligned} \lambda_0 &= 1 - \left(2\gamma + \frac{3}{2} \right) \frac{1}{\rho} \\ s_0 &= \left(\gamma + \frac{3}{4} - \frac{\mu(E_n + 2V_0)}{2\hbar^2 2\alpha} \right) \frac{1}{\rho} \end{aligned}$$

The eigenvalues of the Eq.(41) is obtained as

$$\begin{aligned} \lambda_1 s_0 - s_1 \lambda_0 &= 0 \implies \varepsilon_0 = \alpha \left(\frac{3}{2} + 2\gamma \right) \\ \lambda_2 s_1 - s_2 \lambda_1 &= 0 \implies \varepsilon_1 = \alpha \left(\frac{7}{2} + 2\gamma \right) \\ \lambda_3 s_2 - s_3 \lambda_2 &= 0 \implies \varepsilon_2 = \alpha \left(\frac{11}{2} + 2\gamma \right) \\ &\dots\dots\dots \end{aligned}$$

which can be generalized as

$$\varepsilon_n = \alpha \left[2n + 1 + 2\left(\gamma + \frac{1}{4}\right) \right] \quad (42)$$

where $\varepsilon_n = \frac{\mu(E_n + 2V_0)}{2\hbar^2}$ and n is radial quantum number. The corresponding wavefunctions can be found by using the Eq.(17)

$$\begin{aligned} f_0(\rho) &= 1 \\ f_1(\rho) &= 3 + 4\gamma - 2\rho \\ f_2(\rho) &= 15 + 32\gamma + 16\gamma^2 - 16\gamma\rho - 20\rho + \rho^2 \\ f_3(\rho) &= 105 + 284\gamma + 240\gamma^2 + 64\gamma^3 - 288\gamma\rho - 96\gamma^2\rho - 210\rho + 84\rho^2 + 48\gamma\rho^2 - 8\rho^3 \\ &\dots\dots\dots \end{aligned}$$

from these equations we can write the general formula for $f_n(\rho)$ as Laguerre function

$$f_n(\rho) = L_n^{\frac{1}{2}\sqrt{1+16\sigma}}$$

Now we can find the total radial wavefunction from Eq.(7) by changing the parameters

$$R_{n\ell}(\rho) = \rho^{\frac{1}{4}(-1+\sqrt{1+16\sigma})} \exp\left[-\frac{\rho}{2}\right] L_n^{\frac{1}{2}\sqrt{1+16\sigma}}(\rho) \quad (43)$$

which is exactly as same as with the equation obtained in [35]

V. CONCLUSION

In this study, an alternative method is proposed for the solution of r^{-1} and r^{-2} type potentials of diatomic molecules in Schrödinger equation. The proposed method not only shows compliance with solutions that obtained by the asymptotic iteration method (AIM) but also transform to the second order differential equation form which can be solved by AIM.

By determining the α , β , γ and σ parameters for Mie potential, Kratzer-Fues potential, Coulomb potential, and Pseudoharmonic potential, the corresponding eigenvalues and eigenfunctions are calculated exactly. In addition to satisfying the results in literature, they are obtained very easier than the other solution methods without using complex algebraic calculation.

The proposed method gives the exact solutions only for the specified type potentials. By changing the function in Eq .5, the general form radial equation can be applied to the other potentials such as exponential, trigonometric, etc.

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